

Molecules

Supporting Information

Optimization of alkaloid lappaconitine with pyrimidine motif on the anthranilic acid moiety: Design, synthesis and investigation of antinociceptive potency

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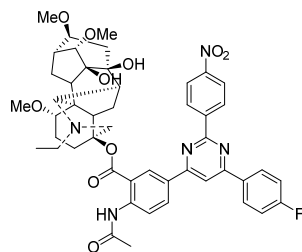
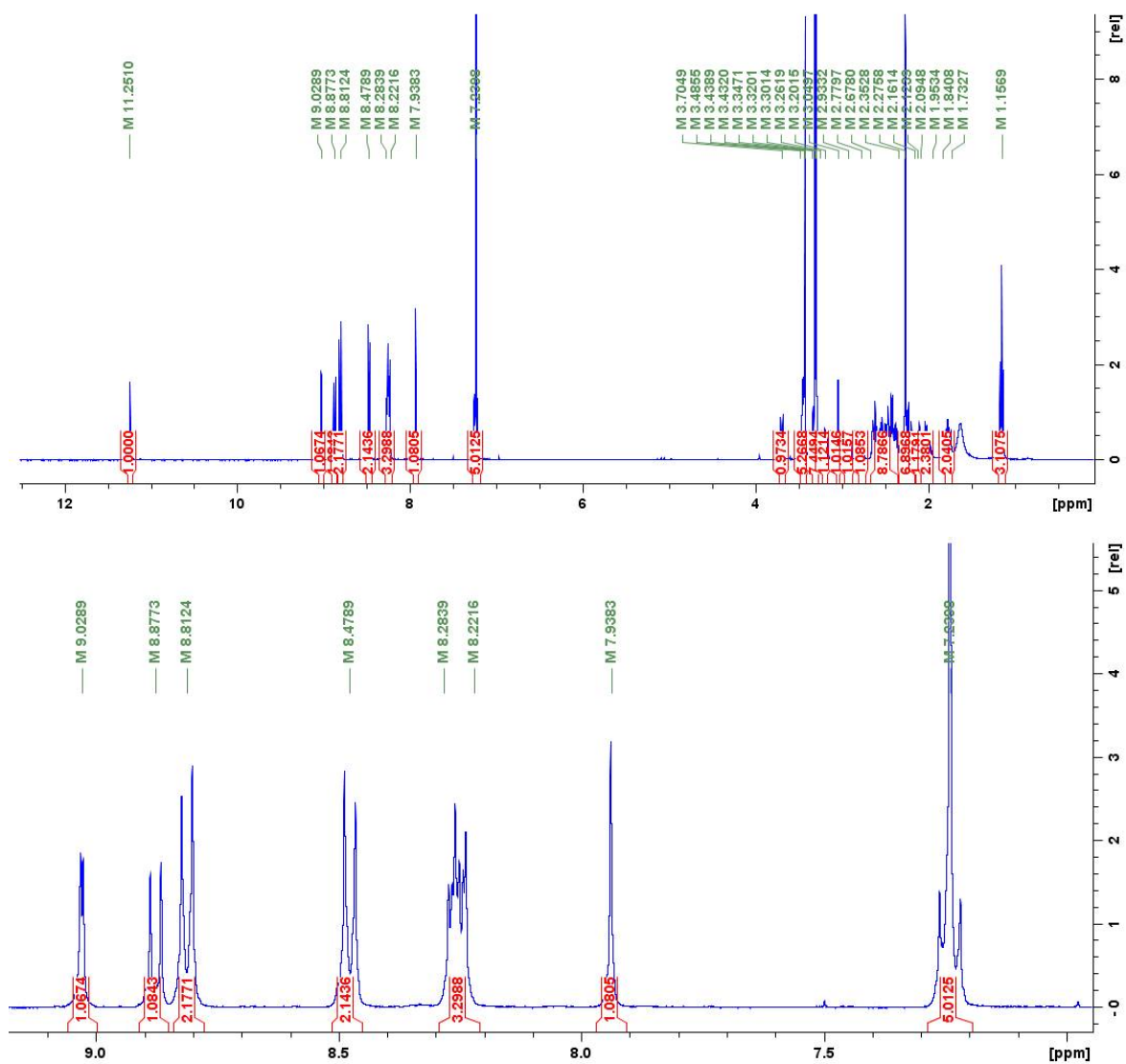
¹H and ¹³C NMR spectra of final compounds.....S2-S13

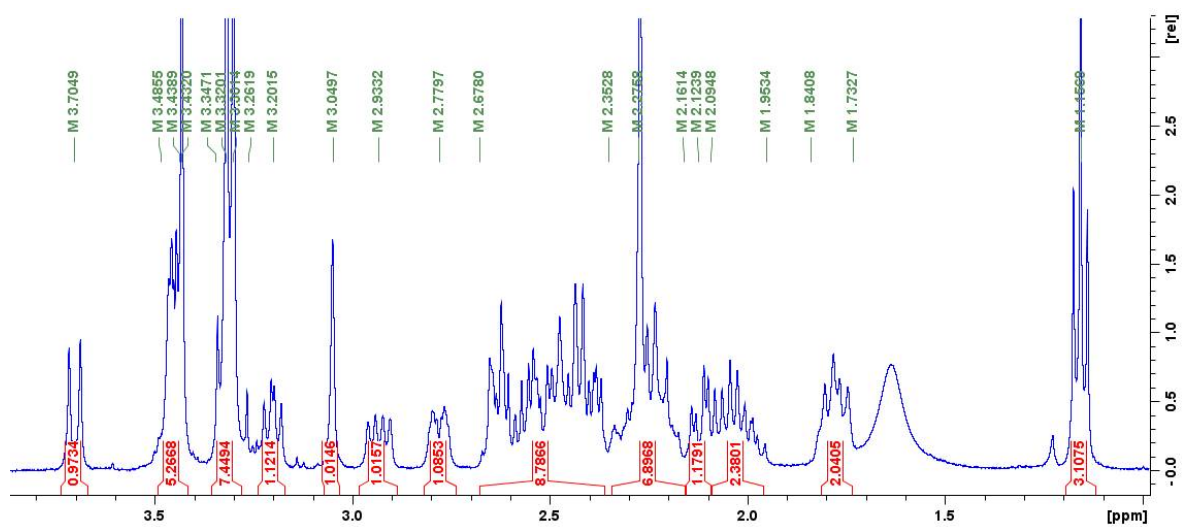
✉ Elvira E. Shults

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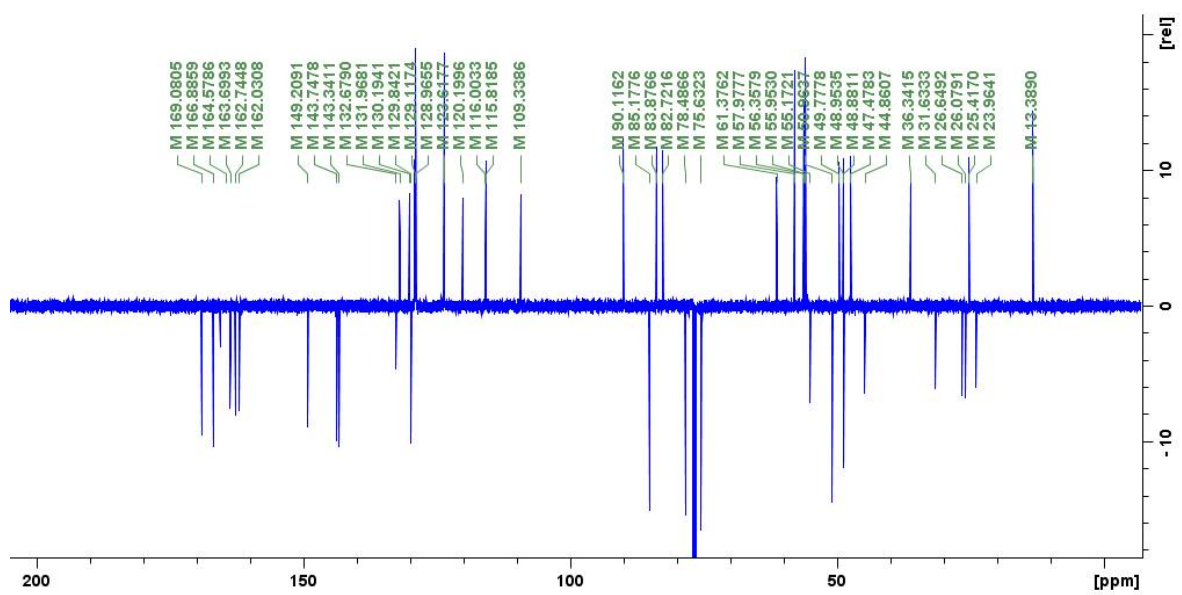
¹ Laboratory of Medicinal Chemistry, Novosibirsk Institute of Organic Chemistry, Siberian Branch of the Russian Academy of Sciences, Lavrentyev Ave, 9, 630090 Novosibirsk, Russia;

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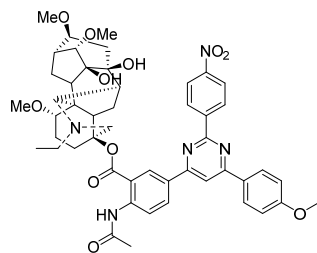
 ^1H NMR (CDCl_3 , 400 MHz)



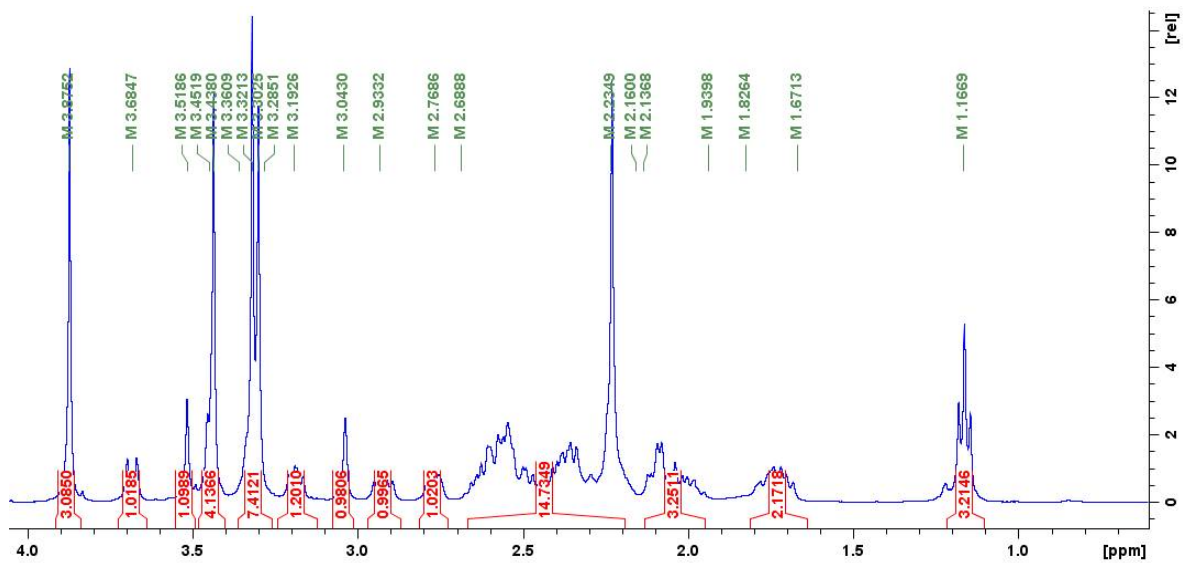
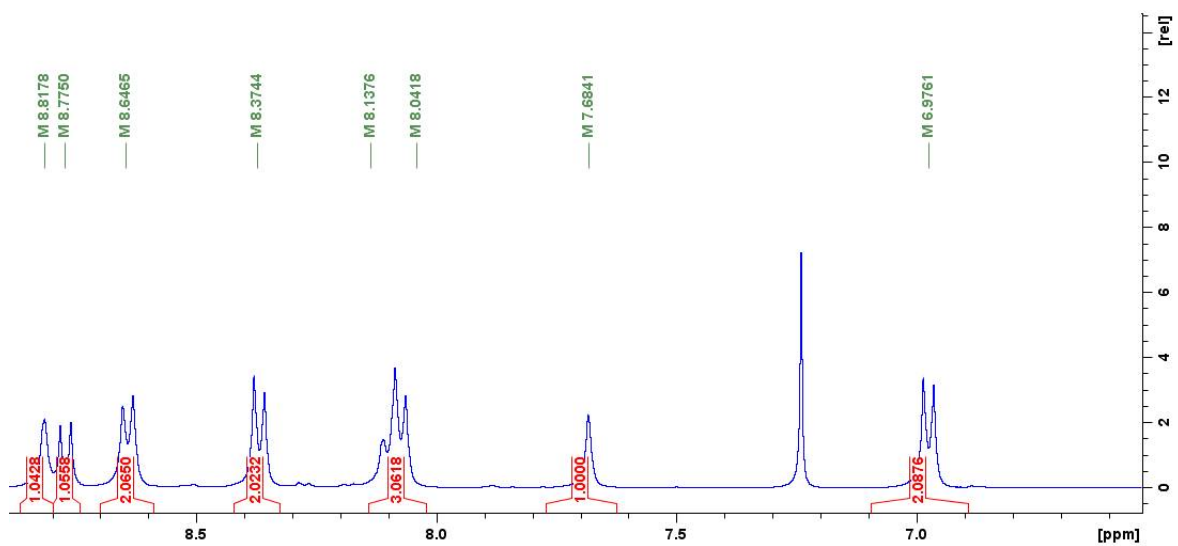
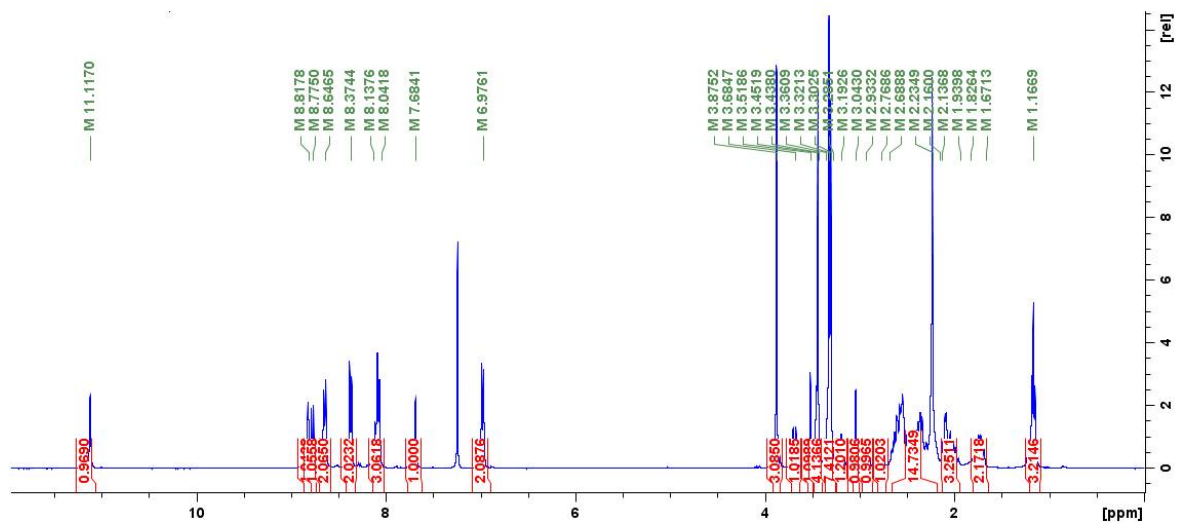
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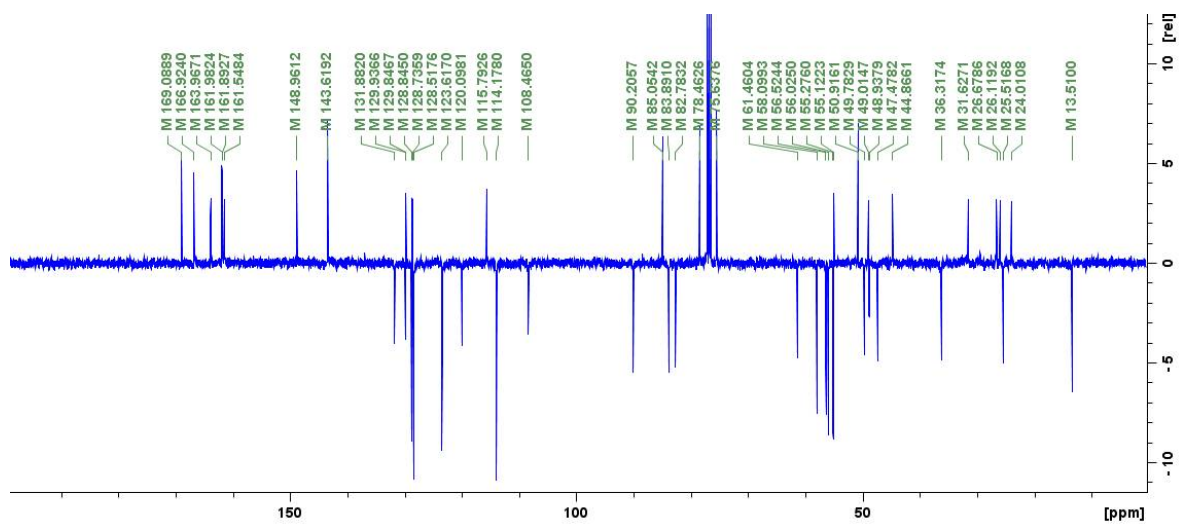
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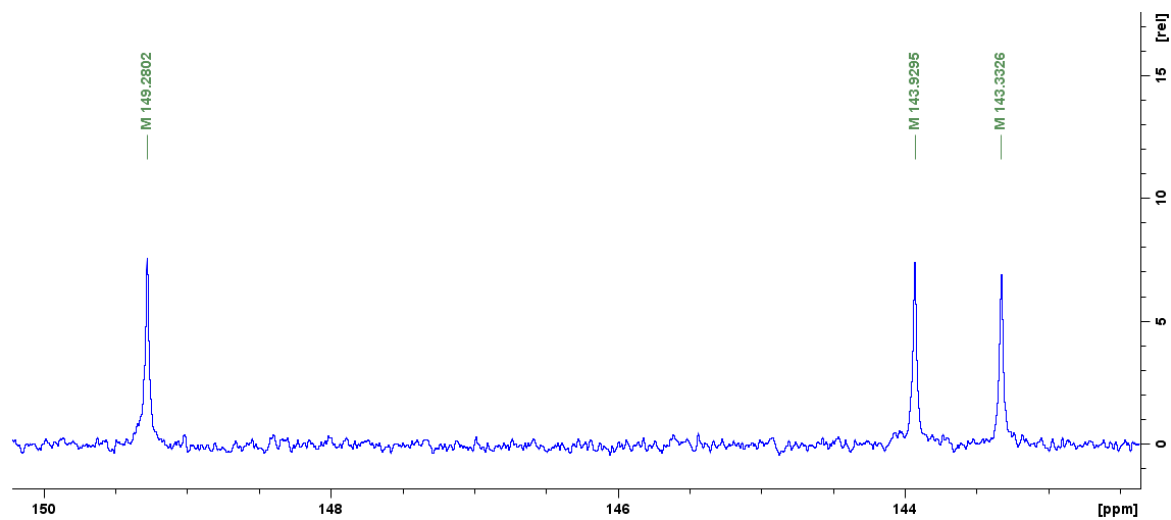
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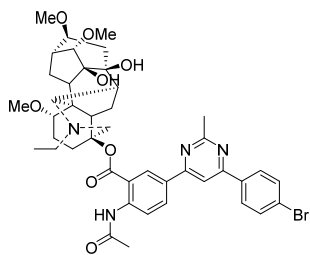
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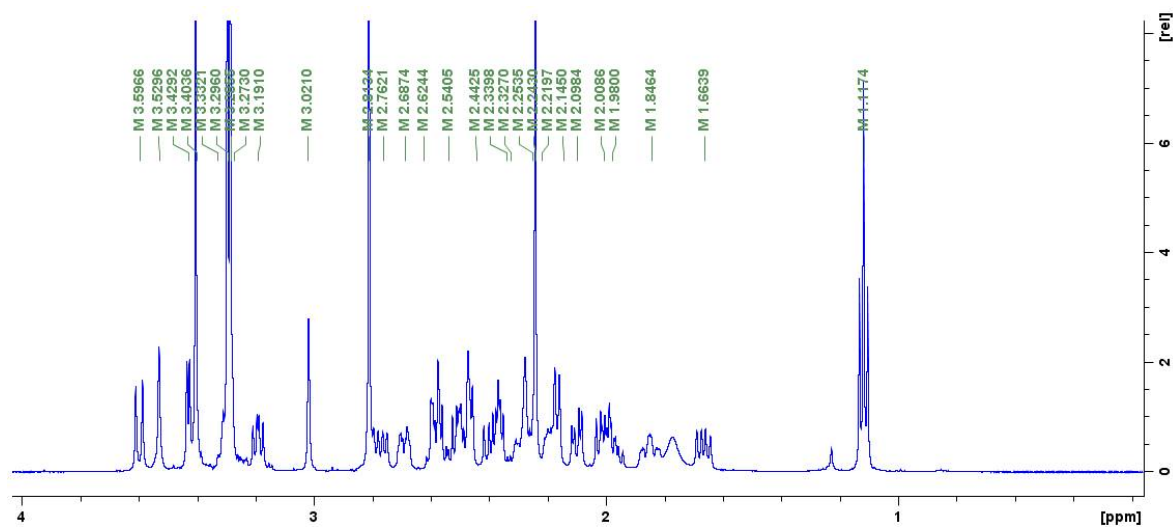
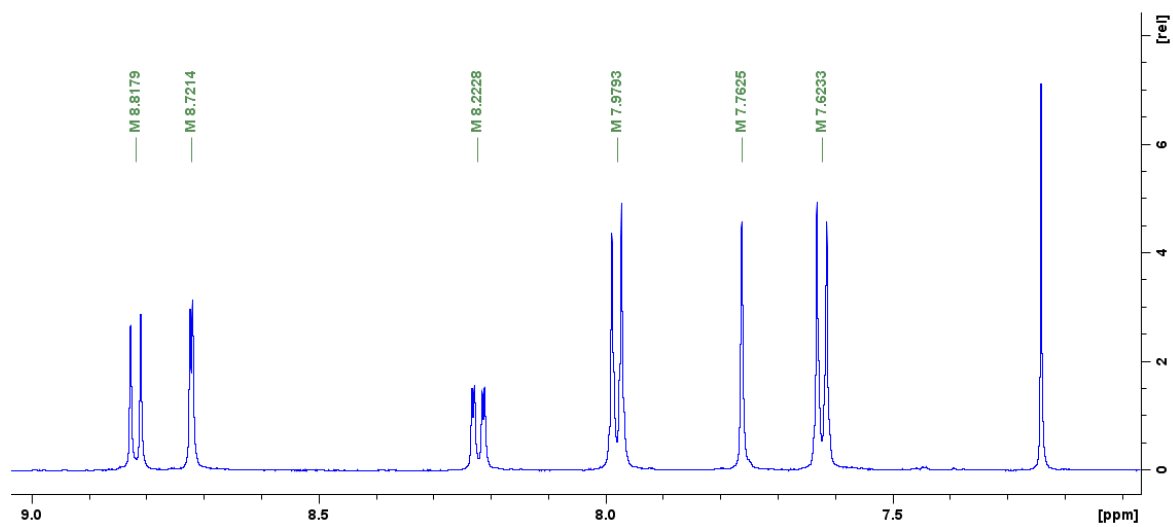
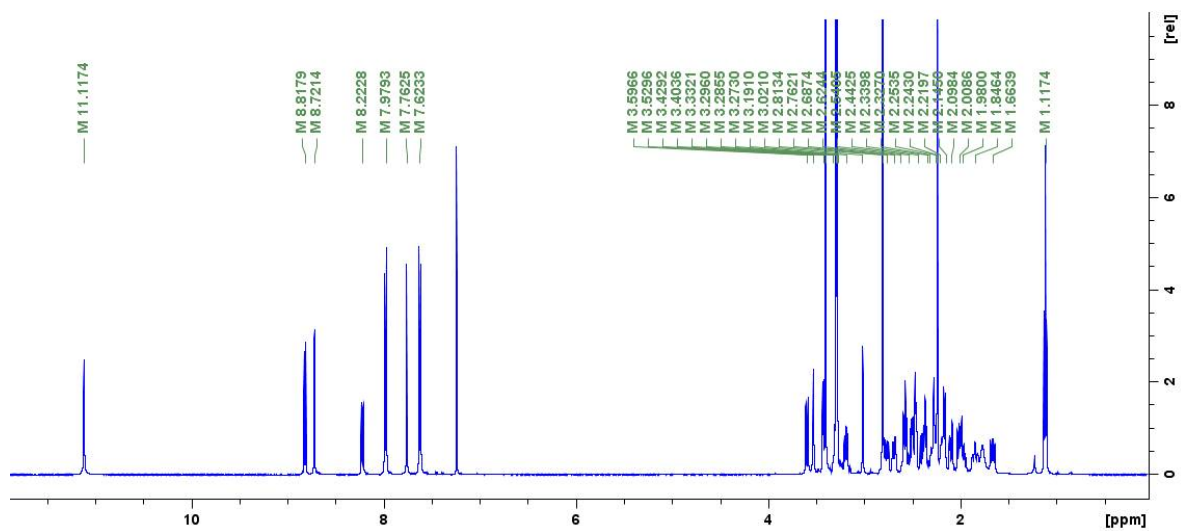
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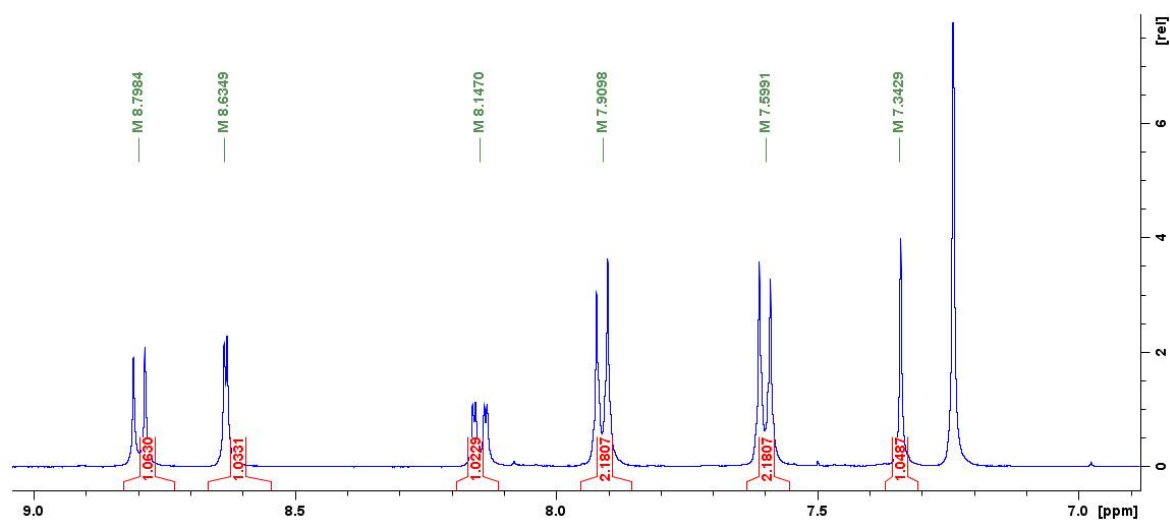
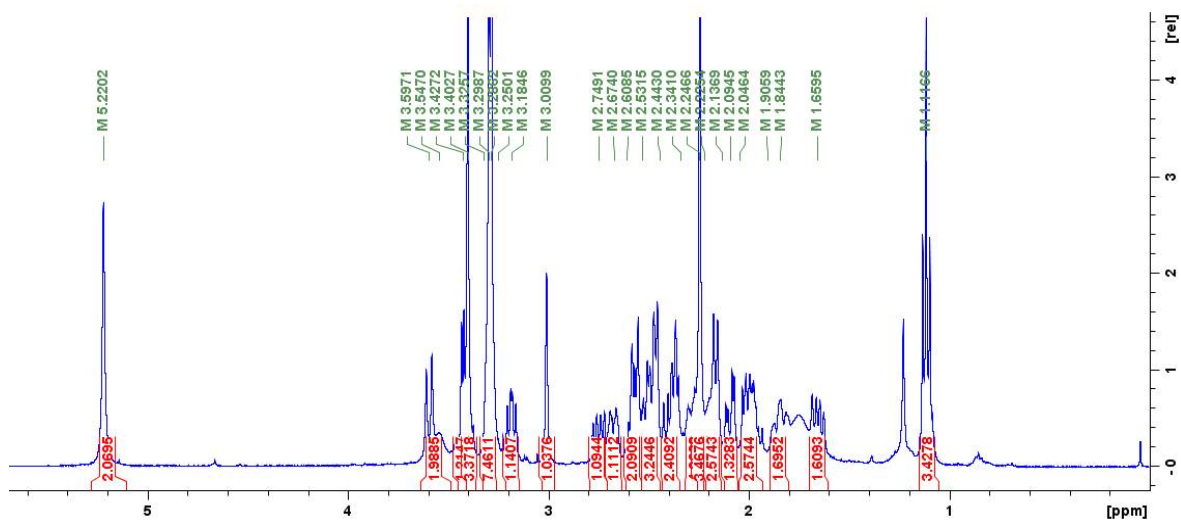
¹H NMR (CDCl₃, 500 MHz)



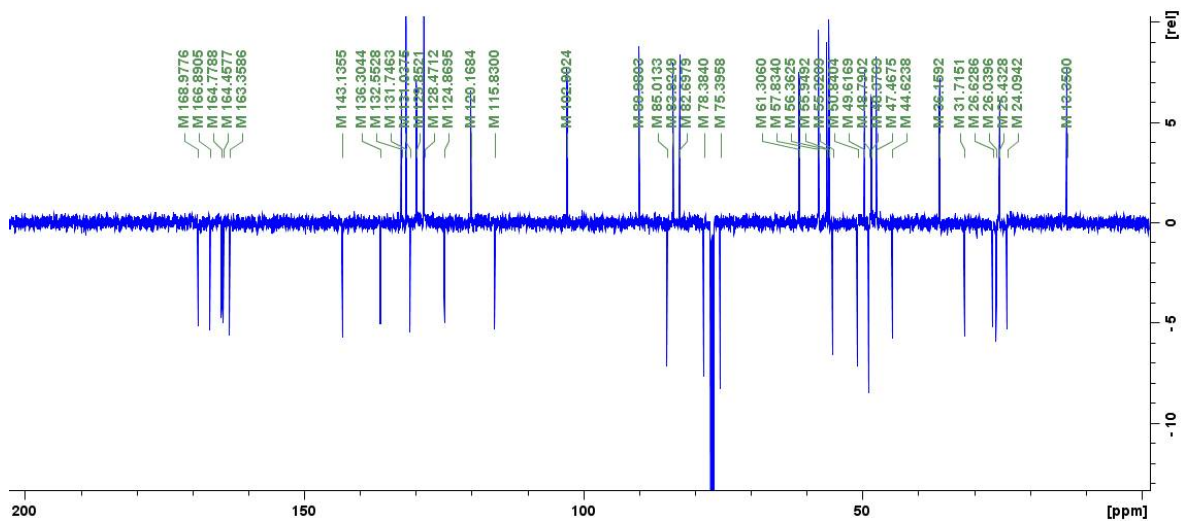
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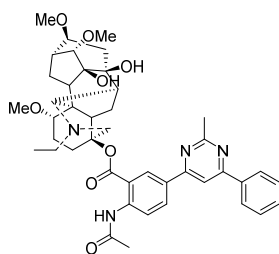
¹H NMR spectrum (CDCl₃) of compound 10. The x-axis represents chemical shift in ppm (0 to 10), and the y-axis represents relative intensity (0 to 10). The spectrum shows several sharp singlet peaks. Integration values are provided below the baseline for each major peak group. Chemical shift values are listed above the peaks.

Chemical Shift (ppm)	Integration
11.1370	1.0000
8.7984	1.0630
8.6349	1.0331
8.1470	1.0223
7.9098	2.1807
7.5991	2.1807
7.3429	1.0487
5.2202	2.0695
3.5971	1.9885
3.5470	3.3716
3.4772	2.4611
3.3272	1.4017
3.3257	1.0376
3.2867	1.9914
3.2501	2.0409
3.1846	3.2749
3.0099	3.2749
2.7491	1.5343
2.6740	1.5343
2.6085	2.5743
2.5115	1.6952
2.4335	1.6952
2.3410	1.6952
2.2466	1.6952
2.2254	1.6952
2.1369	1.6952
2.0945	1.6952
2.0464	1.6952
1.9059	1.6952
1.8443	1.6952
1.6595	1.6952
1.1166	3.4278

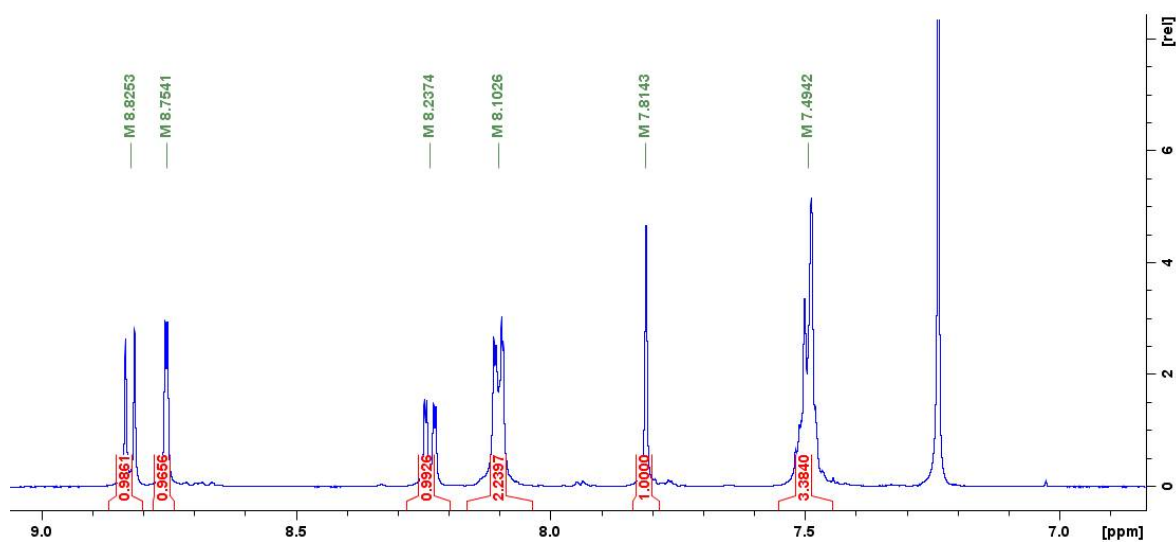
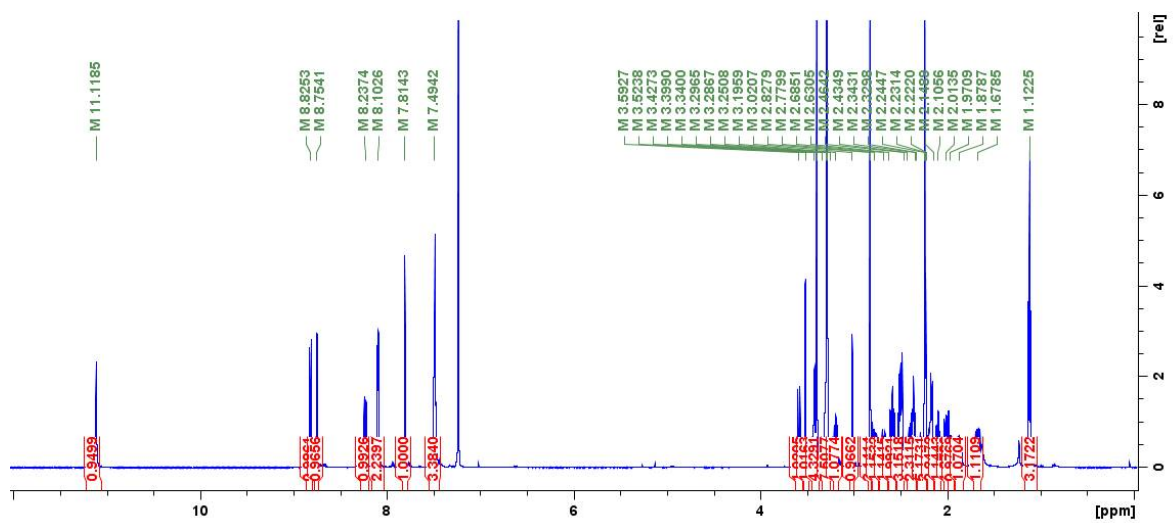


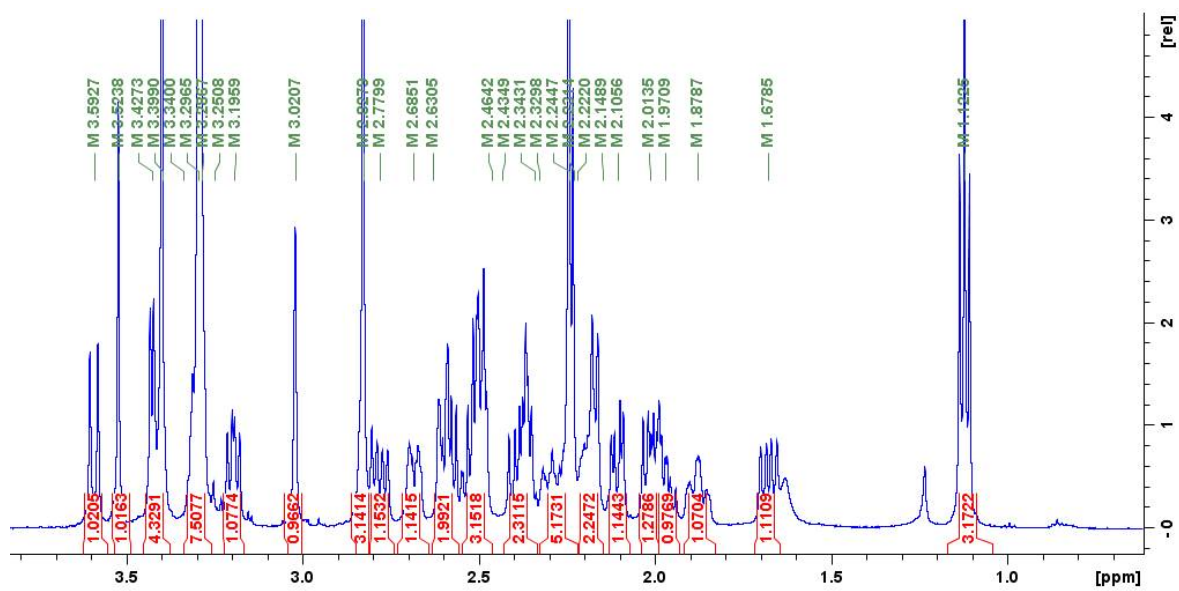
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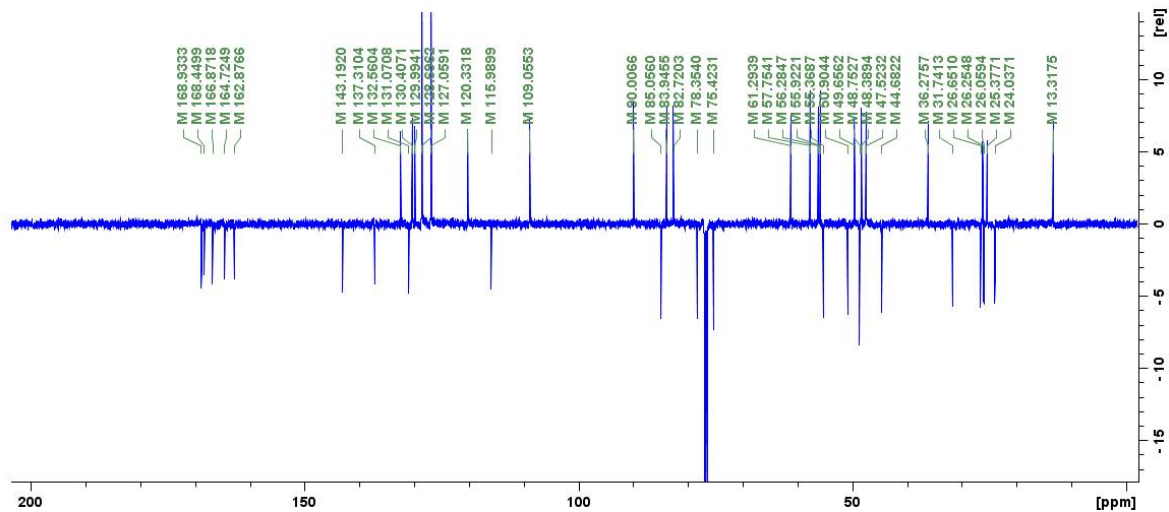


^1H NMR (CDCl_3 , 500 MHz)

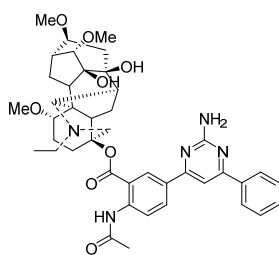




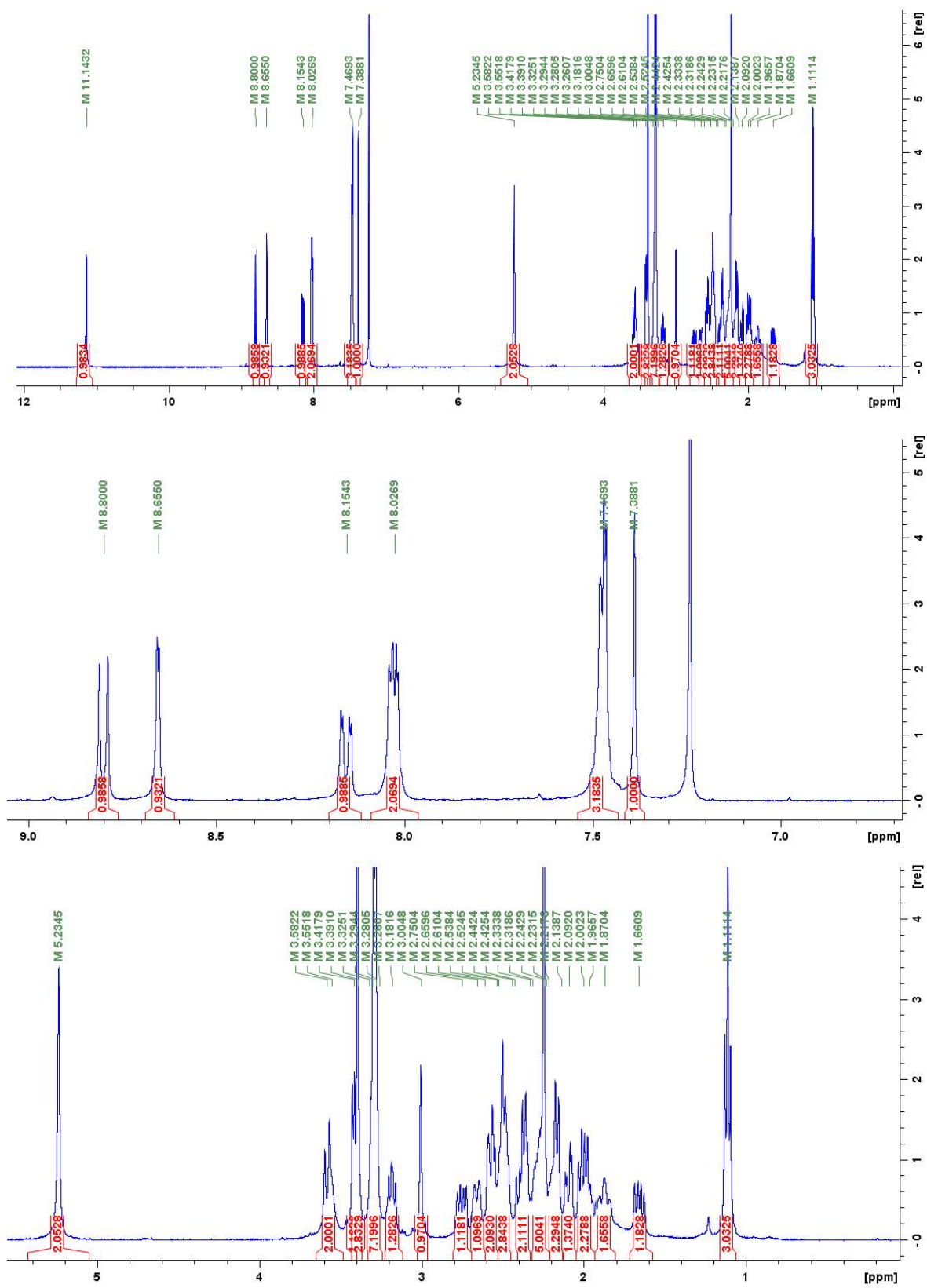
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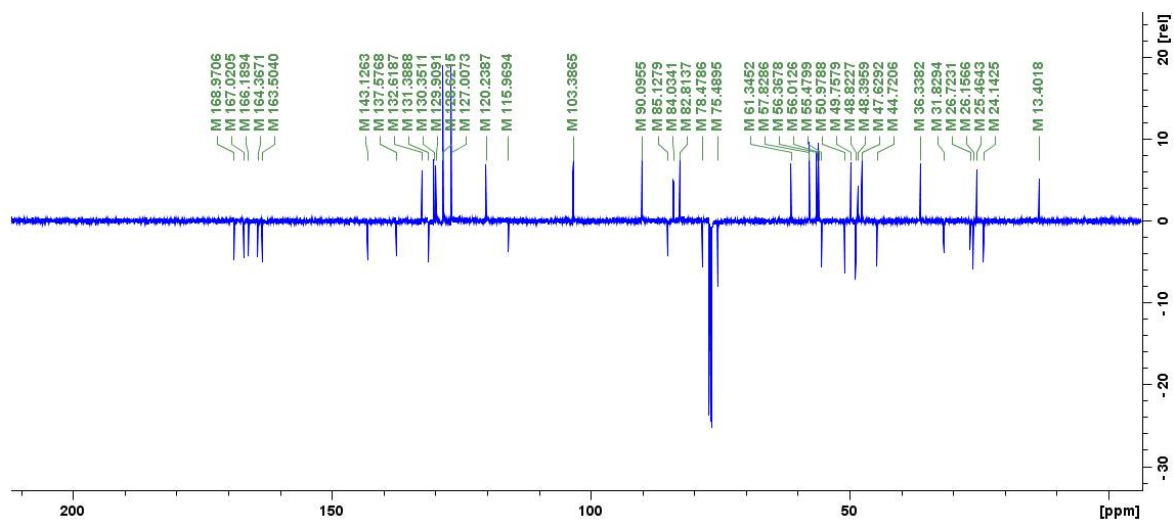
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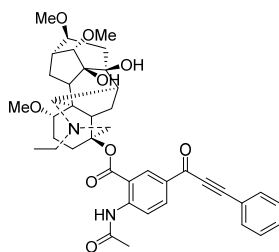
¹H NMR (CDCl₃, 400 MHz)



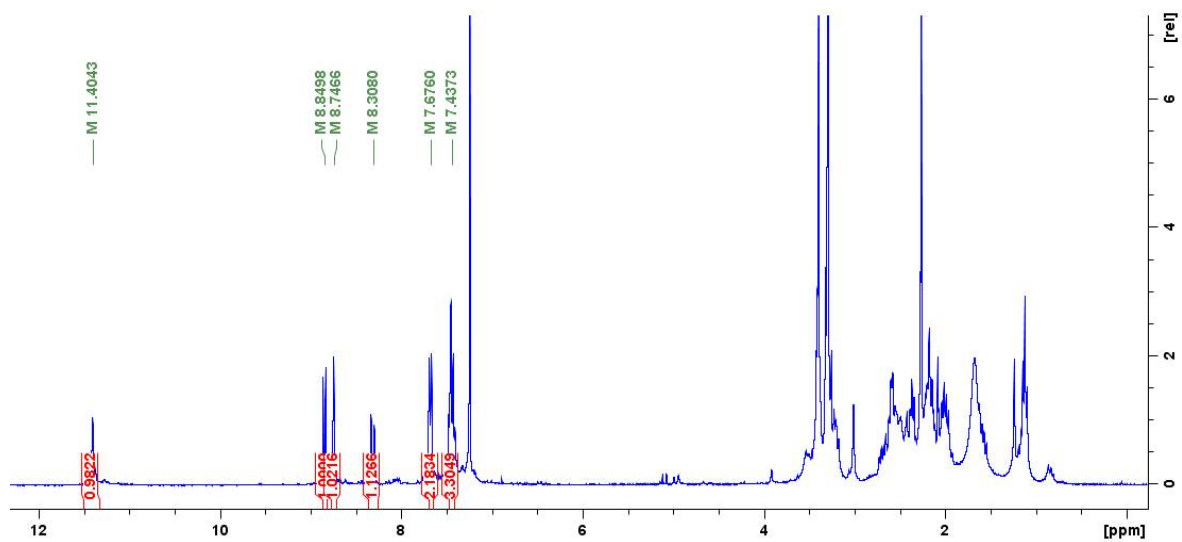
^{13}C NMR (CDCl_3 , 125 MHz)



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¹H NMR (CDCl₃, 300 MHz)



¹³C NMR (CDCl₃, 125 MHz)

